Low- and high-field induced uniform and staggered magnetizations of a spin ladder with DM term

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February 2, 2008

Abstract

Analytic expressions for uniform and staggered magnetizations of a spin ladder with a staggered Dzyaloshinskii-Moriya interaction along rungs are obtained in the lowest perturbative orders. The obtained formulas describe magnetic behavior in two marginal regions related to low ($h \ll h_c$) and high ($h \gg h_s$) magnetic fields.

1 Introduction

Recently a spin ladder model with staggered Dzyaloshinskii-Moriya (DM) term was suggested for explanation of two magnetic anomalies in dimer system $Cu_2(C_5H_{12}N_2)_2Cl_4$ [1],[2],[3]. The first anomaly is an appearance of a staggered magnetization in a uniform magnetic field detected by NMR [1]. The second one is a pronounced smooth behavior of zero temperature magnetization curve near the critical h_c and saturation h_s points [2]. A numerical calculation of these effects within the suggested model produced a good agreement between the theory and experiment [3].

In the present paper we develop an analytical approach to both these problems studying the DM term perturbatively and considering a spin ladder in two different regimes related to vicinities of rung-dimerized and full-polarized ground states. The former corresponds to low magnetic fields $h \ll h_c$. In this case we put the special condition on

the coupling parameters [4],[5] in order to begin with exact rung-dimerized ground state of the nonperturbed Hamiltonian. In the latter regime related to high fields $h \gg h_s$ the unperturbed system is always fully polarized. Therefore in this case any additional restriction on the coupling parameters is unnecessary.

2 Hamiltonian and ground states of a spin ladder

We shall study the following Hamiltonian,

$$\hat{H} = \sum_{n=-\infty}^{\infty} H^0_{n,n+1} + H^{DM}_n, \tag{1}$$

where

$$H^0_{n,n+1} = H^{rung}_{n,n+1} + H^{leg}_{n,n+1} + H^{frust}_{n,n+1} + H^{cyc}_{n,n+1} + H^{Zeeman}_{n,n+1} + J_{norm} I, \tag{2}$$

and

$$\begin{aligned}
H^{rung}_{n,n+1} &= \frac{J_\perp}{2}(\mathbf{S}_{1,n}\cdot\mathbf{S}_{2,n} + \mathbf{S}_{1,n+1}\cdot\mathbf{S}_{2,n+1}),\\
H^{leg}_{n,n+1} &= J_\parallel(\mathbf{S}_{1,n}\cdot\mathbf{S}_{1,n+1} + \mathbf{S}_{2,n}\cdot\mathbf{S}_{2,n+1}),\\
H^{frust}_{n,n+1} &= J_{frust}(\mathbf{S}_{1,n}\cdot\mathbf{S}_{2,n+1} + \mathbf{S}_{2,n}\cdot\mathbf{S}_{1,n+1}),\\
H^{cyc}_{n,n+1} &= J_c((\mathbf{S}_{1,n}\cdot\mathbf{S}_{1,n+1})(\mathbf{S}_{2,n}\cdot\mathbf{S}_{2,n+1}) + (\mathbf{S}_{1,n}\cdot\mathbf{S}_{2,n})(\mathbf{S}_{1,n+1}\cdot\mathbf{S}_{2,n+1})\\
&- (\mathbf{S}_{1,n}\cdot\mathbf{S}_{2,n+1})(\mathbf{S}_{2,n}\cdot\mathbf{S}_{1,n+1})),\\
H^{Zeeman}_{n,n+1} &= -\frac{g\mu_B h}{2}(\mathbf{S}^z_{1,n} + \mathbf{S}^z_{2,n} + \mathbf{S}^z_{1,n+1} + \mathbf{S}^z_{2,n+1}),\\
H^{DM}_n &= (-1)^n \mathbf{D}\cdot[\mathbf{S}_{1,n}\times\mathbf{S}_{2,n}].
\end{aligned} \tag{3}$$

Here $\mathbf{S}_{i,n}$ $(i = 1, 2)$ are spin-1/2 operators associated with n-th rung while I is an identity matrix. The auxiliary term $J_{norm}I$ in (2) is need only for zero normalization of the ground state energy. The vector $\mathbf{D} = D(0, \cos\theta, \sin\theta)$ lies in the $y - z$ plane.

When the coupling parameters of $H^0_{n,n+1}$ satisfy a system of rung-dimerization conditions [4],[5],

$$\begin{aligned}
J_{frust} &= J_\parallel - \frac{1}{2}J_c, \quad J_{norm} = \frac{3}{4}J_\perp - \frac{9}{16}J_c,\\
J_\perp &> 2J_\parallel, \quad J_\perp > \frac{5}{2}J_c, \quad J_\perp + J_\parallel > \frac{3}{4}J_c.
\end{aligned} \tag{4}$$

the ground state related to $H^0_{n,n+1}$ has zero energy and the rung-dimerized form,

$$|0\rangle_{r-d} = \prod_n |0\rangle_n. \tag{5}$$

Here each $|0\rangle_n$ is the singlet state (rung-dimer) related to n-th rung. The related one-particle excitation (often called a *triplon*) is a coherent superposition of excited rungs,

$$|k,tripl\rangle^j = \frac{1}{\sqrt{N}}\sum_n \mathrm{e}^{ikn}...|1\rangle_n^j..., \quad j=-1,0,1, \tag{6}$$

where N is the number of rungs and "..." denotes a product of rung-dimers. The corresponding dispersion is the following [4],

$$E_{tripl}(k,j) = J_\perp - \frac{3}{2}J_c - jg\mu_B h + J_c\cos k. \tag{7}$$

When the external magnetic field satisfy the system of saturation conditions,

$$\begin{aligned} g\mu_B h &> 2(J_\parallel + J_{frust}), \quad g\mu_B h > J_\perp + 2J_{frust}, \quad g\mu_B h > J_\perp + 2J_\parallel + J_c, \\ g\mu_B h &> \frac{J_\perp}{2} + J_\parallel + J_{frust} - \frac{J_c}{4} \\ &+ \frac{1}{2}\sqrt{\Big(J_\perp - J_\parallel - J_{frust} - \frac{J_c}{2}\Big)^2 + 3\Big(J_\parallel - J_{frust} - \frac{J_c}{2}\Big)^2}, \end{aligned} \tag{8}$$

and $J_{norm} = g\mu_B h - J_\perp/4 - J_\parallel/2 - J_{frust}/2 - J_c/16$, the fully polarized state,

$$|0\rangle_{sat} = \prod_n |1\rangle_n^1, \tag{9}$$

is a zero energy ground state for $\hat{H}^0$.

From the local formula,

$$H_n^{DM}|1\rangle_n^+ = (-1)^n\frac{D}{\sqrt{8}}\cos\theta|0\rangle_n, \tag{10}$$

one can conclude that the lowest order with respect to D correction to $|0\rangle_{sat}$ originates from the following branch of coherent excitations (by analogy with (6) we call them *singlons*),

$$|k,singl\rangle = \frac{1}{\sqrt{N}}\sum_n \mathrm{e}^{ikn}...|0\rangle_n... \tag{11}$$

Unlike (6) here "..." denotes a product of polarized rung triplets (with $j=1$).

The corresponding dispersion,

$$E_{singl}(k) = g\mu_B h - J_\perp - J_\parallel - J_{frust} - \frac{J_c}{2} + \Big(\frac{J_c}{2} + J_\parallel - J_{frust}\Big)\cos k, \tag{12}$$

may be easily obtained from the Shrödinger equation and the following local formulas,

$$\begin{aligned}
H^0_{n,n+1}|0\rangle_n|1\rangle^+_{n+1} &= \Big(\frac{g\mu_B h}{2}-\frac{J_\perp}{2}-\frac{J_\parallel}{2}-\frac{J_{frust}}{2}-\frac{J_c}{4}\Big)|0\rangle_n|1\rangle^+_{n+1}\\
&+ \Big(\frac{J_c}{4}+\frac{J_\parallel}{2}-\frac{J_{frust}}{2}\Big)|1\rangle^+_n|0\rangle_{n+1},\\
H^0_{n,n+1}|1\rangle^+_n|0\rangle_{n+1} &= \Big(\frac{g\mu_B h}{2}-\frac{J_\perp}{2}-\frac{J_\parallel}{2}-\frac{J_{frust}}{2}-\frac{J_c}{4}\Big)|1\rangle^+_n|0\rangle_{n+1}\\
&+ \Big(\frac{J_c}{4}+\frac{J_\parallel}{2}-\frac{J_{frust}}{2}\Big)|0\rangle_n|1\rangle^+_{n+1}. \qquad (13)
\end{aligned}$$

3 Magnetization at low fields

In the first order with respect to D the perturbed ground state is the following,

$$|0\rangle = |0\rangle_{r-d} - \sum_{n,k,j}\frac{{}^j\langle k,tripl|H^{DM}_n|0\rangle_{r-d}}{E_{tripl}(k,j)}|k,tripl\rangle^j. \qquad (14)$$

Using the local formula,

$$H^{DM}_n|0\rangle_n = (-1)^n D\Big(\frac{1}{\sqrt{8}}\cos\theta(|1\rangle^+_n+|1\rangle^-_n)+\frac{1}{2i}\sin\theta|1\rangle^0_n\Big), \qquad (15)$$

and taking into account that $\sum_n(-1)^n\mathrm{e}^{-ikn}=N\delta_{k,\pi}$ we obtain,

$$|0\rangle = |0\rangle_{r-d} - D\sqrt{N}\Big(\frac{\cos\theta}{\sqrt{8}}\sum_{j=\pm1}\frac{1}{E_{tripl}(\pi,j)}|\pi,tripl\rangle^j+\frac{\sin\theta}{2iE_{tripl}(\pi,0)}|\pi,tripl\rangle^0\Big). \qquad (16)$$

As it follows from (16) the first order correction diverges as $\sqrt{N}$. Nevertheless as it will be shown below the uniform and staggered magnetizations defined as [3],

$$\begin{aligned}
\mathbf{m}_u(h) &= \langle 0|\mathbf{S}_{1,0}+\mathbf{S}_{2,0}|0\rangle, \qquad (17)\\
\mathbf{m}_s(h) &= \frac{1}{2}\langle 0|\mathbf{S}_{1,0}-\mathbf{S}_{2,0}-\mathbf{S}_{1,1}+\mathbf{S}_{2,1}|0\rangle, \qquad (18)
\end{aligned}$$

remain finite. This phenomena which is rather common for spin systems was also mentioned in [6] where the correct perturbation theory based on cluster expansions was developed. Our naive calculations may be reproduced by this approach.

Using (16) and the following formulas,

$$\begin{aligned}
(\mathbf{S}_{1,n}+\mathbf{S}_{2,n})|0\rangle_n = 0, \quad (\mathbf{S}^z_{1,n}+\mathbf{S}^z_{2,n})|1\rangle^j_n &= j|1\rangle^j_n,\\
[\mathbf{S}^x_{1,n}+\mathbf{S}^x_{2,n}\pm i(\mathbf{S}^y_{1,n}+\mathbf{S}^y_{2,n})]|1\rangle^j_n &= \sqrt{2}|1\rangle^{j\pm1}_n,\\
[\mathbf{S}^x_{1,n}-\mathbf{S}^x_{2,n}\pm i(\mathbf{S}^y_{1,n}-\mathbf{S}^y_{2,n})]|0\rangle_n &= \mp\sqrt{2}|1\rangle^{\pm1}_n,\\
(\mathbf{S}^z_{1,n}-\mathbf{S}^z_{2,n})|0\rangle_n &= |1\rangle^0_n. \qquad (19)
\end{aligned}$$

one obtain,

$$\begin{aligned}
\mathbf{m}_u^x(h) &= 0, \\
\mathbf{m}_u^y(h) &= -\frac{D^2\sin 2\theta}{8E_{gap}}\sum_{j=\pm 1}\frac{j}{E_{gap}-jg\mu_B h}, \\
\mathbf{m}_u^z(h) &= \frac{D^2\cos^2\theta}{8}\sum_{j=\pm 1}\frac{j}{(E_{gap}-jg\mu_B h)^2}, \\
\mathbf{m}_s^x(h) &= \frac{D\cos\theta}{2}\sum_{j=\pm 1}\frac{j}{E_{gap}-jg\mu_B h} \\
\mathbf{m}_s^y(h) &= 0, \quad \mathbf{m}_s^z(h) = 0.
\end{aligned} \tag{20}$$

For $h \ll h_c$ or equivalently $g\mu_B h \ll E_{gap}$ these formulas reduce to a compact form,

$$\begin{aligned}
\mathbf{m}_u(\mathbf{h}) &= \frac{g\mu_B}{2E_{gap}^3}[[\mathbf{D}\times\mathbf{h}]\times\mathbf{D}], \\
\mathbf{m}_s(\mathbf{h}) &= \frac{g\mu_B}{E_{gap}^2}[\mathbf{D}\times\mathbf{h}],
\end{aligned} \tag{21}$$

similar to the one obtained in [3] for a single dimer.

Finitely we notice that though the perturbed ground state (16) is expanded only up to the first order of D, the uniform magnetization is proportional to D^2. In general this result requires also a D^2 term in the expansion for $|0\rangle$ because a matrix element between this term and $|0\rangle_{r-d}$ would be of order D^2. However according to the first formula in the Eq. (19) the latter term always vanishes. Therefore our result is correct.

4 Magnetization at high fields

At high fields it is more convenient to study a deviation of the uniform magnetization from its saturation value $\mathbf{m}_u^{sat} = (0,0,1)$,

$$\Delta\mathbf{m}_u(h) = \mathbf{m}_u^{sat} - \mathbf{m}_u(h). \tag{22}$$

In components,

$$\begin{aligned}
\Delta\mathbf{m}_u^{x,y}(h) &= -\langle 0|\mathbf{S}_{1,0}^{x,y}+\mathbf{S}_{2,0}^{x,y}|0\rangle, \\
\Delta\mathbf{m}_u^{z}(h) &= \langle 0|1-\mathbf{S}_{1,0}^{z}-\mathbf{S}_{2,0}^{z}|0\rangle.
\end{aligned} \tag{23}$$

Both $\Delta\mathbf{m}_u(h)$ and $\mathbf{m}_s(h)$ may be calculated in the same way as in the low-field case. The perturbed ground state,

$$|0\rangle = |0\rangle_{sat} - \frac{D\cos\theta}{\sqrt{8N}}\sum_n(-1)^n\sum_k\frac{\mathrm{e}^{-ikn}}{E_{singl}(k)}|k,singl\rangle^j, \tag{24}$$

reduces to,

$$|0\rangle = |0\rangle_s - \frac{\sqrt{N} D \cos\theta}{\sqrt{8} E_{singl}(\pi)} |\pi, singl\rangle. \tag{25}$$

Substituting this expression into (23) and using (19), we obtain,

$$\begin{aligned}
\Delta \mathbf{m}_u^x(h) &= \Delta \mathbf{m}_u^y(h) = 0, \quad \Delta \mathbf{m}_u^z(h) = \frac{D^2 \cos^2\theta}{8 E_{singl}^2(\pi)}, \\
\mathbf{m}_s^x(h) &= \frac{D \cos\theta}{2 E_{singl}(\pi)}, \quad \mathbf{m}_s^y(h) = \mathbf{m}_s^z(h) = 0.
\end{aligned} \tag{26}$$

As a consequence of (26),

$$\Delta \mathbf{m}_u^z(h) = \frac{1}{2} (\mathbf{m}_s^x(h))^2. \tag{27}$$

As it follows from (26) polarization for $D \neq 0$ reaches the saturation value only asymptotically. Therefore the saturation field h_s strictly speaking has a sense only for the free Hamiltonian $\hat{H}^0$ and is defined as the minimal field satisfying all the inequalities in (8).

At a high magnetic field $h \gg h_s$ taking in account (12) one can reduce the system (26) as follows,

$$\begin{aligned}
\Delta \mathbf{m}_u^z(h) &= \frac{D^2 \cos^2\theta}{8 g^2 \mu_B^2 h^2} \Big(1 + 2 \frac{J_\perp + 2 J_\parallel + J_c}{g \mu_B h}\Big), \\
\mathbf{m}_s^x(h) &= \frac{D \cos\theta}{2 g \mu_B h} \Big(1 + \frac{J_\perp + 2 J_\parallel + J_c}{g \mu_B h}\Big).
\end{aligned} \tag{28}$$

5 Conclusion

In the first order with respect to the staggered DM term we obtained analytical expressions for the uniform and staggered magnetizations at low (21) and high (28) magnetic fields. The corresponding magnetization experiment was reported in [7]. Although the presented plot well reproduces a global behavior of the magnetic curve between h_c and h_s the representation in the marginal regions $h \ll h_c$ and $h \gg h_s$ is rather crude for comparison with the formulas (21) and (28). Therefore we refrain from any estimations for D basing on the data presented in [7].

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